

Hexachloroethane
67-72-1 | DTXSID7020689

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 118 °C

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 3.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hexachloroethane</div> <div>Measured: 187</div> <div>Predicted: 118</div>	<div>Image not found</div> <div>Hexachloropropene</div> <div>Measured: -72.9</div> <div>Predicted: -34.7</div>	<div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: -22.3</div> <div>Predicted: -13.3</div>
<div>Image not found</div> <div>Carbon tetrachloride</div> <div>Measured: -23.0</div> <div>Predicted: -3.94</div>	<div>Image not found</div> <div>Hexachloro-1,3-butadiene</div> <div>Measured: -21.0</div> <div>Predicted: -20.7</div>	